LOCV calculations for polarized liquid ^{3}He with the spin-dependent correlation

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Abstract

We have used the lowest order constrained variational (LOCV) method to calculate some ground state properties of polarized liquid ^3He at zero temperature with the spin-dependent correlation function employing the Lennard-Jones and Aziz pair potentials. We have seen that the total energy of polarized liquid ^3He increases by increasing polarization. For all polarizations, it is shown that the total energy in the spin-dependent case is lower than the spin-independent case. We have seen that the difference between the energies of spin-dependent and spin-independent cases decreases by increasing polarization. We have shown that the main contribution of the potential energy comes from the spin-triplet state.

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I. INTRODUCTION

Helium has two stable isotopes: that of mass 4 is readily available as helium gas or liquid from the atmosphere or gas wells, while that of mass 3 is extremely rare in nature and only became available commercially in the 1950s [1]. Liquid ^3He is particularly suited to study correlation among the strongly interacting many-body fermionic systems. Several approaches have been used for investigating the properties of normal liquid ^3He. These are mainly based on the STLS scheme [2], mott localization [3], spin fluctuation theory [4], Green's function Monte Carlo (GFMC) [5], FN-DMC, DMC, VMC and EMC simulations [6], CBPT formalism [7], nonperturbative renormalization group equation [8], nonlocal density functional formalism [9] , correlated basis functions (CBF) [10] and Fermi hyper-netted chain (FHNC) [11]. The spin polarized liquid ^3He as an interesting many-body system has been investigated using different approaches such as FHNC [12], GFMC [13], CBF [14] and transport theory [15].

In recent years, we have studied both normal and polarized liquid ^3He at zero and finite temperature [16, 17, 18, 19]. In these calculations, the lowest order constrained variational (LOCV) method based on the cluster expansion of the energy functional has been used. This method is fully self-consistent, since it does not introduce any free parameter to the calculations. We have also used the LOCV method in many-body calculations of dense matter [20]. Recently, we have used this method to calculate some properties of the polarized neutron matter and the polarized symmetrical and asymmetrical nuclear matters [21]. In these works, a comparison of our results and those of other many-body techniques indicates that the LOCV method is a powerful microscopic technique to calculate the properties of the polarized matter.

In this work, we use the LOCV method to compute the ground state energy of the polarized liquid ^3He at zero temperature by employing the spin-dependent correlation function with the Lennard-Jones [22] and Aziz [23, 24] pair potentials.

II.   LOWEST ORDER CONSTRAINED VARIATIONAL METHOD

We consider a system of N interacting ^3He atoms with N^+ spin up and N^- spin down atoms. The total number density (ρ) and spin asymmetry parameter (ξ) are defined as

$$\rho = \rho^+ + \rho^-,$$
$$\xi = \frac{N^+ - N^-}{N}. \tag{1}$$

ξ shows the spin ordering of matter which can have a value in the range of $\xi = 0.0$ (unpolarized matter) to $\xi = 1.0$ (fully polarized matter). For this system, we consider the energy per particle up to the two-body term in the cluster expansion,

$$E = E_1 + E_2, \tag{2}$$

where

$$E_1 = \frac{3}{10}\frac{\hbar^2}{m}(3\pi^2\rho)^{\frac{2}{3}}[(1+\xi)^{\frac{5}{3}} + (1-\xi)^{\frac{5}{3}}],$$
$$E_2 = \frac{1}{2N}\sum_{i,j}\langle ij \mid w(12) \mid ij - ji\rangle. \tag{3}$$

In the above equation, $w(12)$ is the effective pair potential,

$$w(12) = -\frac{\hbar^2}{2m}[F(12), [\nabla^2_{12}, F(12)]] + F(12)V(12)F(12), \tag{4}$$

where $F(12)$ is the two-body correlation operator and $V(12)$ is the pair potential between the helium atoms. In our calculations, we use the Lennard-Jones [22] and Aziz [23, 24] pair potentials. The Lennard-Jones pair potential is as follows [22],

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right], \tag{5}$$

where

$$\epsilon = 10.22K, \qquad \sigma = 2.556A \cdot \tag{6}$$

The Aziz pair potential has the following form [23, 24],

$$V(r) = \epsilon\left\{Ae^{-\alpha r/r_m} - \left[C_6\left(\frac{r_m}{r}\right)^6 + C_8\left(\frac{r_m}{r}\right)^8 + C_{10}\left(\frac{r_m}{r}\right)^{10}\right]F(r)\right\}, \tag{7}$$

where

$$F(r) = \begin{cases} e^{-(\frac{Dr_m}{r}-1)^2} & ; \frac{r}{r_m} \leq D \\ 1 & ; \frac{r}{r_m} > D, \end{cases} \tag{8}$$

and

$$\frac{\epsilon}{k_B} = 10.8K, \qquad A = 0.5448504 \times 10^6,$$
$$\alpha = 13.353384, \qquad r_m = 2.9673A,$$
$$C_6 = 1.37732412, \qquad C_8 = 0.4253785,$$
$$C_{10} = 0.178100, \qquad D = 1.241314 \cdot$$

$$(9)$$

Now, we consider a spin-dependent correlation function as follows

$$F(12) = f_0(r_{12})P_0 + f_1(r_{12})P_1, \tag{10}$$

where

$$
\begin{aligned}
P_0 &= \frac{1}{4}(1 - \sigma_1 . \sigma_2), \\
P_1 &= \frac{1}{4}(3 + \sigma_1 . \sigma_2).
\end{aligned}
\tag{11}
$$

f_0 and f_1 indicate the spin-singlet and spin-triplet two-body correlation functions, respectively. With the above two-body correlation function, we have derived the following relation for the effective pair potential,

$$w_s(r) = \frac{\hbar^2}{m}(f_s{}'(r))^2 + f_s^2(r)V(r), \tag{12}$$

and then the two-body energy E_2 is found by

$$E_2 = 2\pi\rho \sum_{s=0,1} \int_0^\infty dr r^2 w_s(r) a_s. \tag{13}$$

In Eq. (13)

$$
\begin{aligned}
a_0 &= \frac{1}{4}(1 - \xi^2)[1 + l(k_{F+}r)l(k_{F-}r)], \\
a_1 &= \frac{1}{4}[(1 + \xi)^2(1 - l^2(k_{F+}r)) + (1 - \xi)^2(1 - l^2(k_{F-}r)) \\
&\quad + (1 - \xi^2)(1 - l(k_{F+}r)l(k_{F-}r))].
\end{aligned}
\tag{14}
$$

$k_{F\pm} = (6\pi^2\rho^\pm)^{\frac{1}{3}}$ is the Fermi momentum and $l(x)$ is given by

$$l(x) = \frac{3}{x^3}[\sin(x) - x\cos(x)]. \tag{15}$$

Now, we minimize the two-body energy Eq. (13) with respect to the variations in the two-body correlation function subject to the normalization constraint [25],

$$\frac{1}{N}\sum_{i,j}\langle ij|h^2(12) - F^2(12)|ij - ji\rangle = 1. \tag{16}$$

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The normalization constraint is conveniently re-written in the integral form as

$$4\pi\rho \sum_{s=0,1} \int_0^\infty dr r^2 [h^2(r) - f_s^2(r)]a_s = 1, \tag{17}$$

where the Pauli function $h(r)$ is

$$h(r) = \{1 - \frac{1}{4}[(1+\xi)^2 l^2(k_{F+}r) + (1-\xi)^2 l^2(k_{F-}r)]\}^{-\frac{1}{2}}. \tag{18}$$

The minimization of the two body energy E_2 gives the following Euler-Lagrange differential equation for the two-body correlation function $f_s(r)$,

$$f_s''(r) + (\frac{2}{r} + \frac{a_s'}{a_s})f_s'(r) - \frac{m}{\hbar^2}(V(r) - 2\lambda) = 0. \tag{19}$$

The Lagrange multiplier λ imposes by normalization constraint. For $s = 0$ and $s = 1$ states, the two-body correlation function $f_s(r)$ is obtained by numerically integrating Eq. (19). Using this two-body correlation function we can determine the effective pair potential $w_s(r)$ as a function of interatomic distance from Eq. (12). Finally, the two-body energy E_2 and the total energy of system can be calculated.

III.   RESULTS AND DISCUSSION

We have calculated some ground state properties of the polarized liquid ^3He at zero temperature with the Lennard-Jones [22] and Aziz [23, 24] pair potentials using the spin-dependent correlation function. Our results are as follows.

The spin-dependent two-body correlation functions at $s = 0$ state and $s = 1$ states for different values of spin asymmetry parameter (ξ) are shown in Fig. 1. These figures show that the correlation function at $s = 1$ state heals to pauli function, $h(r)$, more rapidly than $s = 0$ state. Therefore, the $s = 1$ state has a shorter correlation length with respect to $s = 0$ state. For large values of r, $f_0(r)$ and $f_1(r)$ have the same values and therefore, the spin-dependent part of correlation operator (Eq. 10) is vanished. In these figures, the spin-independent two-body correlation function are also plotted for comparison. It is seen that the spin-dependent correlation function differs from spin-independent correlation function, except for the fully polarized matter ($\xi = 1.0$). This is due to the fact that for fully polarized matter, there is only $s = 1$ state. From Fig. 1, we can see that the correlation functions with the Lennard-Jones and Aziz potentials are nearly identical.

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In Fig. 2, we have shown the total energy of polarized liquid ^3He versus number density calculated both with the spin-dependent correlation and the spin-independent correlation at different values of spin asymmetry parameter ξ. We can see that the total energy increases by increasing ξ. Fig. 2 indicates that in the spin-dependent case, the total energy of the liquid ^3He is lower than the spin-independent case. It is also seen that for all values of ξ, the energy curve has a minimum which shows the existence of a bound state for this system. It is shown that the difference between the energies of spin-dependent case and spin-independent case decreases by increasing ξ and it becomes zero as ξ approaches to one. It is seen that for all values of the density and spin asymmetry parameter, the total energy with the Aziz pair potential is grater than that of the Lennard-Jones pair potential.

The potential energy of the polarized liquid ^3He for different values of ξ are presented in Fig. 3, for spin-dependent and spin-independent cases. This figure indicates that the potential energy decreases by increasing the polarization. According to the above results, we can conclude that the increasing of kinetic energy dominates and this leads to the increasing of total energy by increasing ξ. Fig. 3 shows that the potential energy in the spin-dependent case has lower values with respect to the spin-independent case. It is also seen that the difference between the potential energies of spin-dependent and spin-independent cases decrease by increasing ξ. We see that the potential energies with the Aziz and the Lennard-Jones pair potentials are different. This difference increases by increasing the density.

In Fig 4, the potential energies of $s = 0$ and $s = 1$ states for different values of ξ are compared. We have seen that the potential energy at $s = 1$ state is lower than at $s = 0$ state. It can be concluded that the spin-triplet state has the main contribution in the potential energy of polarized liquid ^3He. It is also seen that the potential energy of $s = 0$ ($s = 1$) state increases (decreases) by increasing ξ. For $s = 0$ state, we can see that at low densities, the potential energies with the Lennard-Jones and Aziz pair potentials are nearly identical. However, for $s = 1$ state and high densities, the difference between these potential energies becomes appreciable.

The equation of state of polarized liquid ^3He, $P(\rho, \xi)$, can be obtained using

$$P(\rho, \xi) = \rho^2 \frac{\partial E(\rho, \xi)}{\partial \rho} \tag{20}$$

In Fig. 5, we have presented the pressure of liquid ^3He as a function of the density (ρ) for fully polarized ($\xi = 1.0$) and unpolarized ($\xi = 0.0$) cases. This figure shows that for different

values of the polarization, the equations of state of liquid ^3He are nearly identical. From Fig. 5, it is seen that for both $\xi = 1.0$ and $\xi = 0.0$, the equation of state with the Aziz pair potential is stiffer than that of the Lennard-Jones pair potential.

IV. SUMMARY AND CONCLUSION

We have considered a system consisting of Helium atoms (^3He) with asymmetrical spin configuration and derived the two-body term in the cluster expansion of the energy functional by employing spin-dependent correlation function. Then, we have minimized the two-body energy term under the normalization constraint and obtained the Euler-Lagrange differential equation. By numerically solving this differential equation, we have computed the correlation function and then calculated the other properties of this system with the Lennard-Jones and Aziz pair potentials. It is shown that for the two different spin-singlet and spin-triplet states, the correlation functions are different from each other. Our results show that the introduction of the spin-dependent term in the correlation operator reduces the total energy of system by about 10%. It is also shown that the total energy increases by increasing the polarization. The difference between the energies of the spin-dependent and spin-independent cases decreases by increasing the polarization. We have seen that, the potential energy of these states have a remarkable difference. It is shown that the main contribution of the potential energy comes from $s = 1$ state. Our calculations show that there is a difference between the results with the Lennard-Jones and Aziz pair potentials, especially at high densities.

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[1] E. R. Dobbs, *Helium Three*, (Oxford University Press, 2000).

[2] N. Nafari and A. Doroudi, *Phys. Rev.* **B51**, 9019 (1995).

[3] A. Georges and L. Laloux, *Cond-mat*/961076.

[4] S. G. Mishra and P. A. Streeram, *Cond-mat*/9801042.

[5] R. M. Panoff and J. Carlson, *Phys. Rev. Lett.* **62**, 1130 (1989)

[6] J. Casulleras and J. Boronat,*Phys. Rev. Lett.* **84**, 3121 (2000); S. Moroiny, G. Senatore and S. Fantoni, *Cond-mat*/9608134; S. Moroiny, S. Fantoni and G. Senatore *Phys. Rev.* **B52**, 13547 (1995); S. A. Vitiello, K. E. Schmidt, *Phys. Rev.* **B46**, 5442 (1992).

[7] S. Fantoni, V. R. Pandharipande and K. E. Schmidt, *Phys. Rev. Lett.* **48**, 878 (1982).

[8] M. Kindermann and C. Wetterich, *Cond-mat*/0008332

[9] L. Pricaupenko and J. Treiner, *Phys. Rev. Lett.* **74**, 430 (1995).

[10] E. Krotscheck and R. A. Smith, *Phys. Rev.* **B27**, 4222 (1983); B. L. Friman and E. Krotescheck *Phys. Rev. Lett.* **49**, 1705 (1982).

[11] E. Krotscheck, *J. Low. Temp. Phys.* **44**, 103 (2000); F. Arias de Saaverda and E. Buendiʼa, *Phys. Rev.* **B46** 13934 (1992); M. Takano and M. Yamada, *Prog. Theor. Phys.* **91**, 1149 (1994); J. C. Owen, *Phys. Rev.* **B23**, 2169 (1981).

[12] E. Manousakis, S. Fantoni, V. R. Pandharipande and Q. N. Usmani, *Phys. Rev.* **B28**, 3770 (1983).

[13] D. Levesque, *Phys. Rev.* **B21**, 5159 (1980); C. Lhuillier and D. Levesque, *ibid.* **B23**, 2203 (1981).

[14] E. Krotescheck, J. W. Clark and A. D. Jakson, *Phys. Rev.* **B28**, 5088 (1983).

[15] D. W. Hess and K. F. Quader, *Phys. Rev.* **B36**, 756 (1987).

[16] G. H. Bordbar, M.J. Karimi and J. Vahedi, *Int. J. Mod. Phys.* **B27** (2008) in press.

[17] G. H. Bordbar, S. M. Zebarjad, M. R. Vahdani and M. Bigdeli, *Int. J. Mod. Phys.* **B19**, 3379 (2005).

[18] G.H. Bordbar, S. M. Zebarjad and F. Shojaei, *Int. J. Theor. Phys.* **43**, 1863 (2004).

[19] G. H. Bordbar and M. Hashemi, *Int. J. Theor. Phys., Group Theory and Nonlinear Optics* **8**, 251 (2002).

[20] G. H. Bordbar, *Int. J. Theor. Phys.* **43**, 399 (2004); *ibid.* **41**, 309 (2002); **41**, 1135 (2002); G. H. Bordbar and N. Riazi, *ibid.* **40**, 1671 (2001); G. H. Bordbar, *Int. J. Mod. Phys.* **A18**, 2629 (2003). G. H. Bordbar and M. Modarres, *Phys. Rev* **C57**, 714 (1998); *J. Phys. G: Nucl. Part. Phys.* **23**, 1631 (1997).

[21] G. H. Bordbar and M. Bigdeli, *Phys. Rev* **C77**, 015805 (2008); *ibid.* **C76**, 035803 (2007); **C75**, 045804 (2007).

[22] J. de Boer and A. Michels, Physica **6**, 409 (1939).

[23] R. A. Aziz et al., J. Chem. Phys. **70**, 4330 (1979).

[24] R. A. Aziz, F. R. W. McCourt and C. C. K. Wong, Mol. Phys. **61**, 1487 (1987).

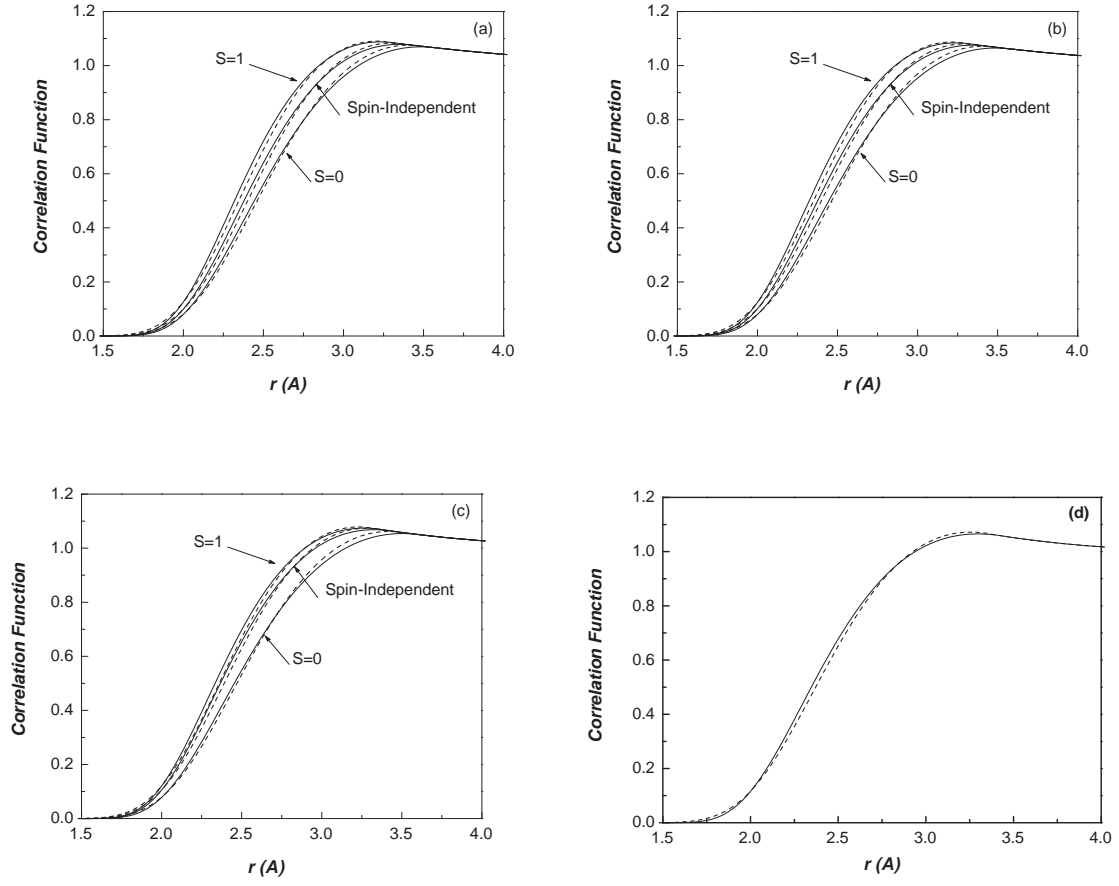[25] J. W. Clark, *Prog. Part. Nucl. Phys.* **2**, 89 (1979).

FIG. 1: The correlation function with the Aziz (dashed curves) and Lennard-Jones (full curves) pair potentials in the case of spin-dependent at $s = 0$ and $s = 1$ states for $\xi = 0.0$ (a), $\xi = 0.33$ (b), $\xi = 0.66$ (c) and $\xi = 1.0$ (d). Our results for the spin-independent correlation function are also presented for comparison.
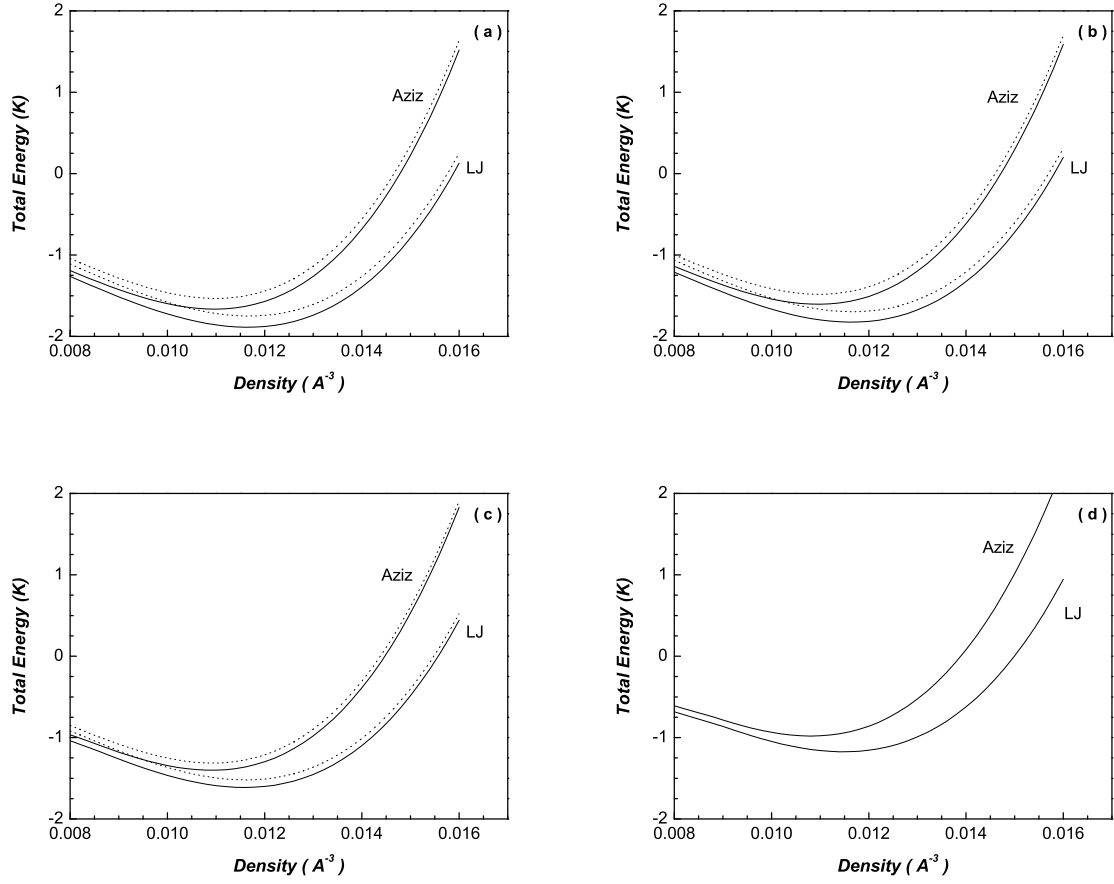
FIG. 2: Our results for the total energy of the polarized liquid ^3He with the Aziz and Lennard-Jones (LJ) pair potentials in the case of spin-dependent (full curve) and spin-independent (dotted curve) correlation functions for $\xi = 0.0$ (a), $\xi = 0.33$ (b), $\xi = 0.66$ (c) and $\xi = 1.0$ (d).
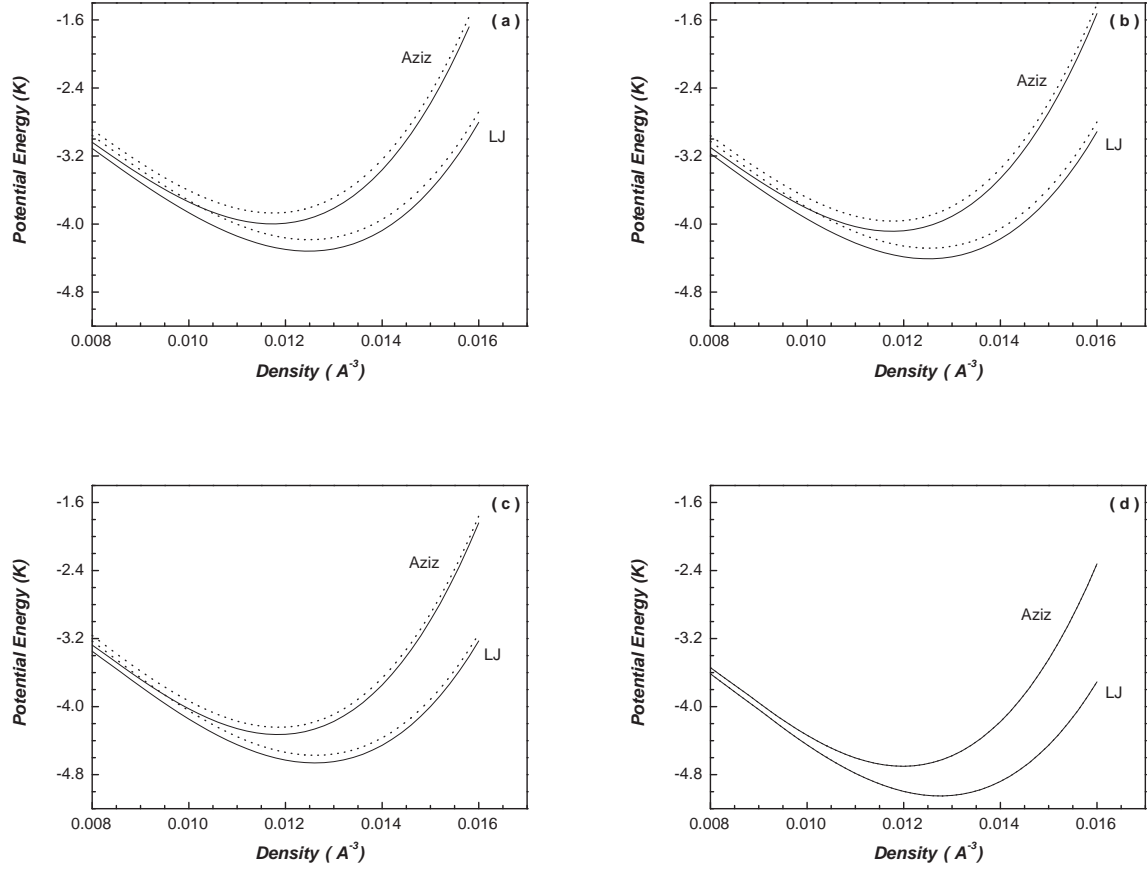
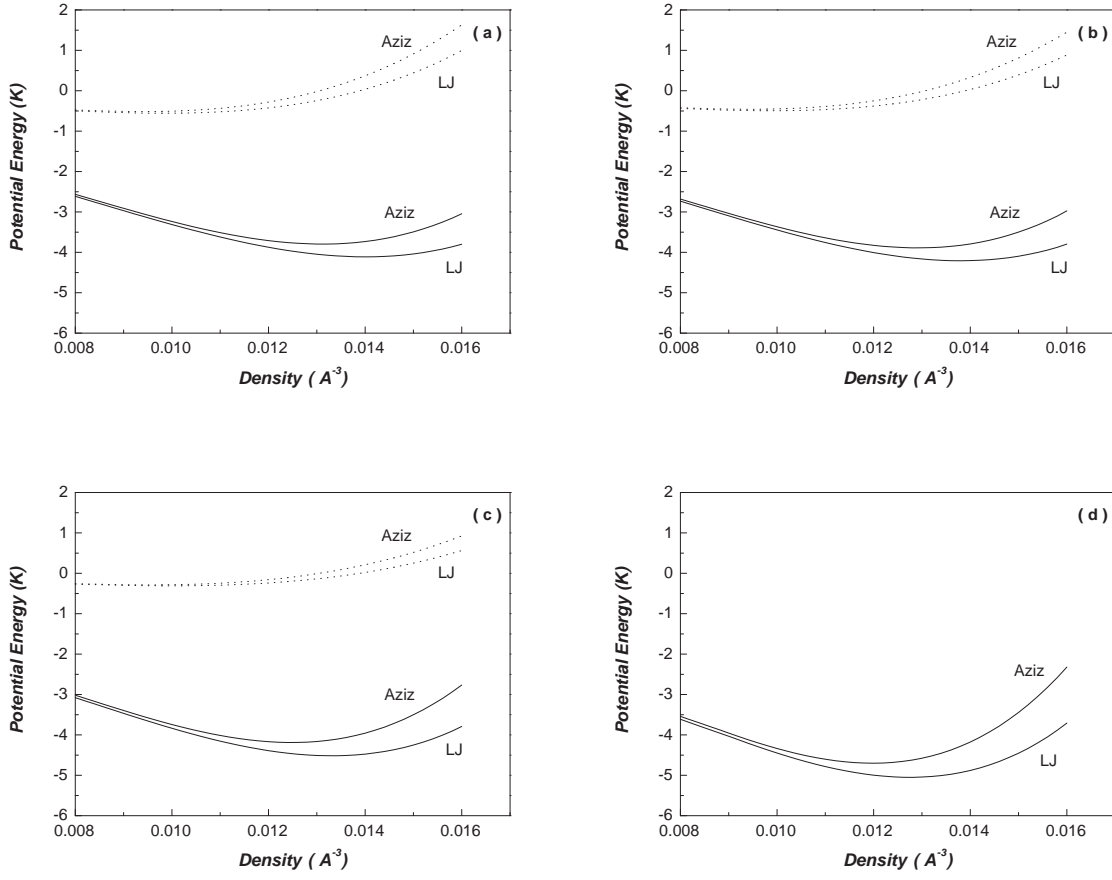FIG. 3: As Fig. 2, but for the potential energy of the polarized liquid ^3He.

FIG. 4: Our results for the potential energy of the polarized liquid ^3He with the Aziz and Lennard-Jones (LJ) pair potentials at $s = 0$ (dotted curve) and $s = 1$ (full curve) states for $\xi = 0.0$ (a), $\xi = 0.33$ (b), $\xi = 0.66$ (c) and $\xi = 1.0$ (d).
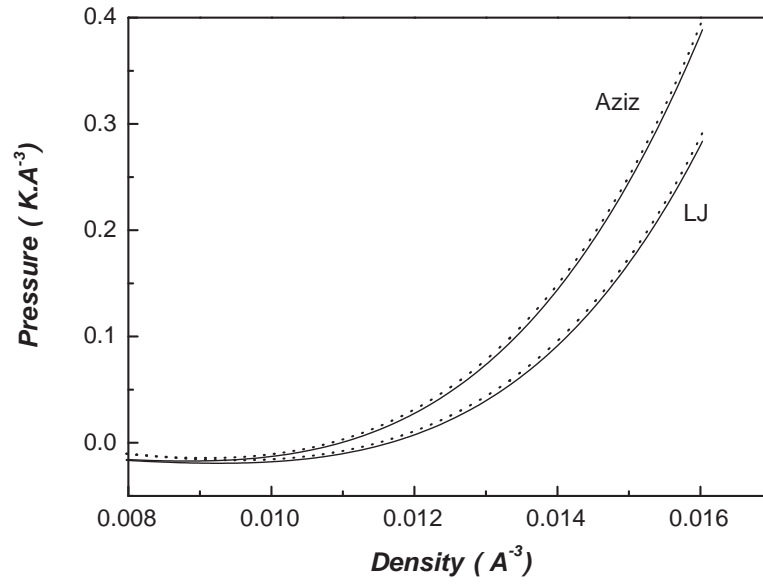
FIG. 5: The equation of state of the fully polarized (dotted curve) and unpolarized (full curve) liquid ^3He with the Aziz and Lennard-Jones (LJ) pair potentials.